MASS CODING FLOWCHART

FIG. 1A

39

GENERATE ALL SUBSETS OF K PERIPHERAL
MOIETY PRECURSORS AND CALCULATE THE
MASS REDUNDANCIES OF THE RESULTANT
LIBRARIES. PASS ONLY THOSE SUBSETS OF K
PERIPHERAL MOIETIES THAT YIELD MASS
CODED LIBRARIES

35

APPLY MASS CODING
ALGORITHMS

33

CHEMISTS SELECT INITIAL SET
OF J PERIPHERAL MOIETY PRECURSORS

31

ALL AVAILABLE PERIPHERAL
MOIETY PRECURSORS

37

COMPUTER SELECTED SET OF
PERIPHERAL MOIETY PRECURSORS

41

SUBSET OF K PERIPHERAL MOIETY
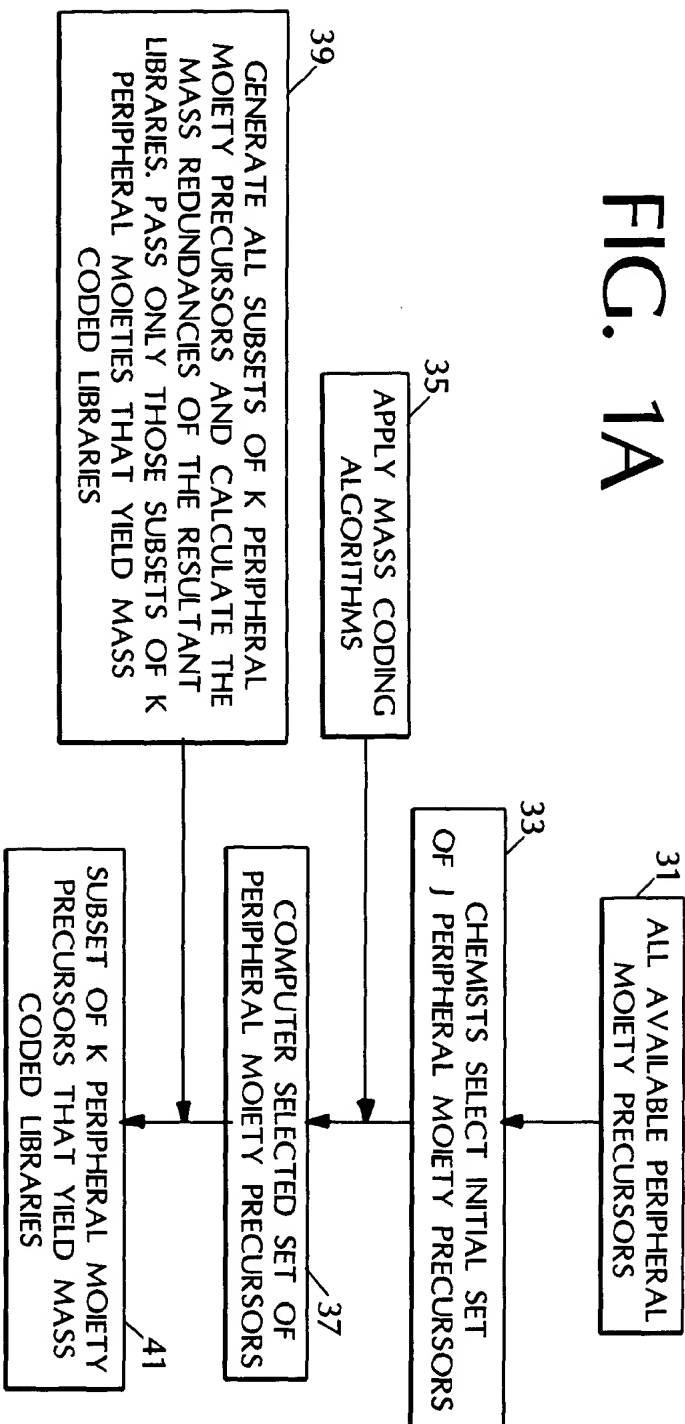PRECURSORS THAT YIELD MASS
CODED LIBRARIES

Appln No.: 09/373,018
Applicant(s): Huw M. Nash, et al.
METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
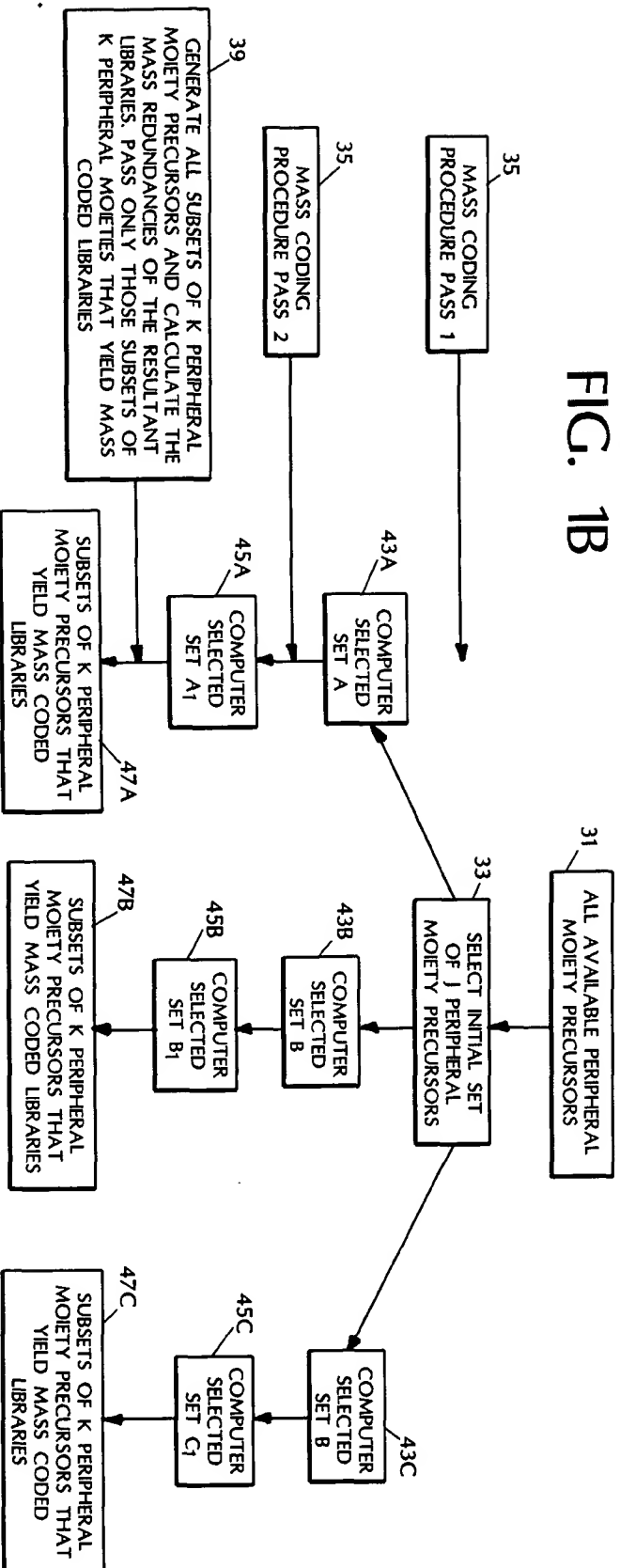DISCOVERY AND TARGET VALIDATION

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ALTERNATE METHOD FOR MASS CODING

FIG. 1B

31 — ALL AVAILABLE PERIPHERAL MOIETY PRECURSORS

33 — SELECT INITIAL SET OF J PERIPHERAL MOIETY PRECURSORS

35 — MASS CODING PROCEDURE PASS 1

35 — MASS CODING PROCEDURE PASS 2

39 — GENERATE ALL SUBSETS OF K PERIPHERAL MOIETY PRECURSORS AND CALCULATE THE MASS REDUNDANCIES OF THE RESULTANT LIBRARIES. PASS ONLY THOSE SUBSETS OF K PERIPHERAL MOIETIES THAT YIELD MASS CODED LIBRARIES

43A — COMPUTER SELECTED SET A

45A — COMPUTER SELECTED SET A₁

47A — SUBSETS OF K PERIPHERAL MOIETY PRECURSORS THAT YIELD MASS CODED LIBRARIES

43B — COMPUTER SELECTED SET B

45B — COMPUTER SELECTED SET B₁

47B — SUBSETS OF K PERIPHERAL MOIETY PRECURSORS THAT YIELD MASS CODED LIBRARIES

43C — COMPUTER SELECTED SET B

45C — COMPUTER SELECTED SET C₁

47C — SUBSETS OF K PERIPHERAL MOIETY PRECURSORS THAT YIELD MASS CODED LIBRARIES

Appln No.: 09/373,018
Applicant(s): Huw M. Nash, et al.
METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
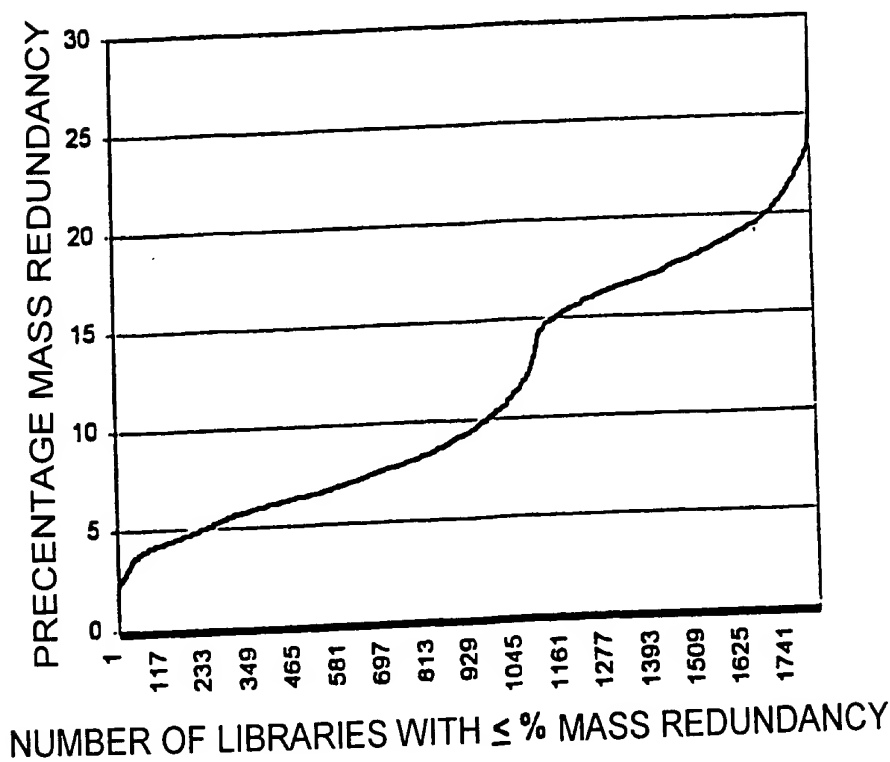DISCOVERY AND TARGET VALIDATION

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% MASS REDUNDANCY OF LIBRARIES FROM A COMPUTER SELECTED SET OF PERIPHERAL MOIETY PRECURSORS

Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	24	1.32
<5%	234	12.86
<10%	972	53.41

Average Mass Redundancy	11.47 Percent

FIG. 2A

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METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
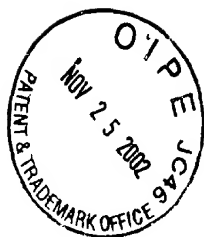DISCOVERY AND TARGET VALIDATION

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% MASS REDUNDANCY OF LIBRARIES
FROM A RANDOMLY CHOSEN SET OF
PERIPHERAL MOIETY PRECURSORS

Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	0	0.00
<5%	0	0.00
<10%	0	0.00

Average Mass Redundancy	60.69 Percent

FIG. 2B

Appln No.: 09/373,018
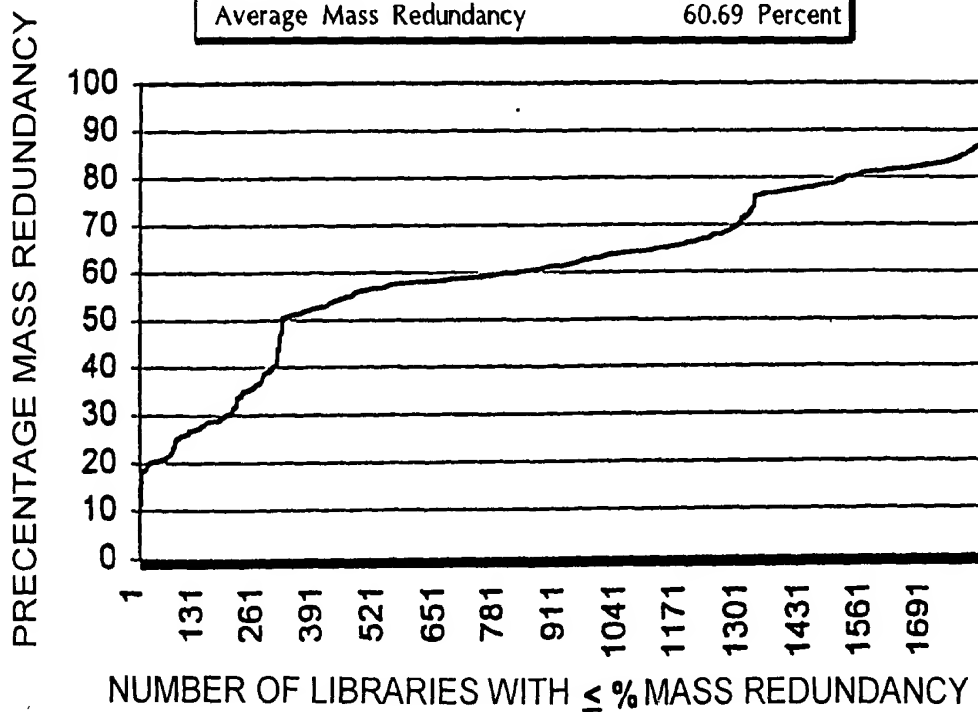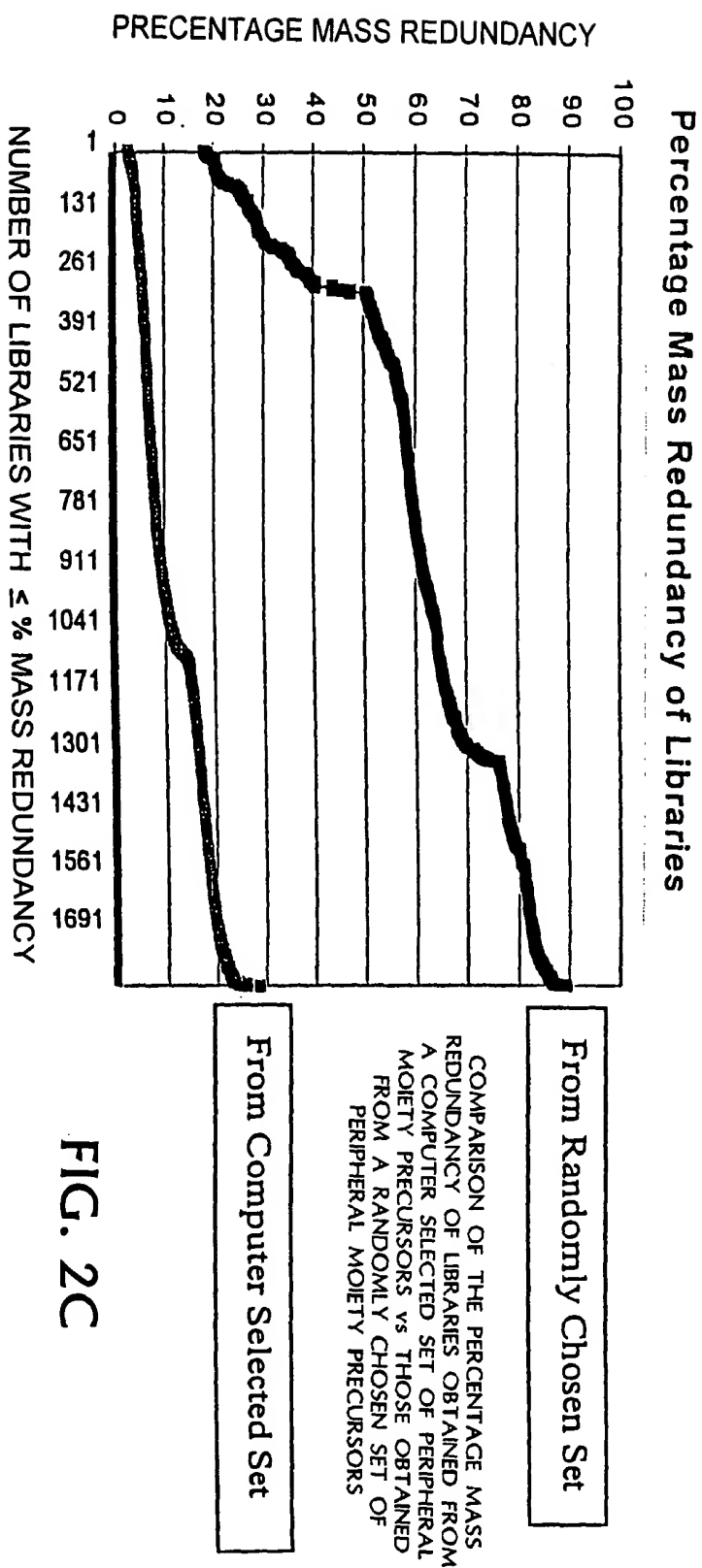Applicant(s): Huw M. Nash, et al.
METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
DISCOVERY AND TARGET VALIDATION

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PRECENTAGE MASS REDUNDANCY

Percentage Mass Redundancy of Libraries

NUMBER OF LIBRARIES WITH ≤ % MASS REDUNDANCY

From Randomly Chosen Set

COMPARISON OF THE PERCENTAGE MASS
REDUNDANCY OF LIBRARIES OBTAINED FROM
A COMPUTER SELECTED SET OF PERIPHERAL
MOIETY PRECURSORS vs THOSE OBTAINED
FROM A RANDOMLY CHOSEN SET OF
PERIPHERAL MOIETY PRECURSORS

From Computer Selected Set

FIG. 2C

13 — PERIPHERAL MOIETY
PRECURSORS STORED IN DATABASE
OR ELECTRONIC DATA STORAGE SYSTEM

COMPUTER SELECTS
FOR USER SET
CRITERIA, DIVERSITY,
SIZE, SHAPE, ETC.

19

15 — HUMAN SELECTION
(VIA 21)

INPUT₁

INITIAL SET OF PERIPHERAL
MOIETY PRECURSORS STORED
IN COMPUTER OR ELECTRONIC
DATA STORAGE SYSTEM
29

11

OUTPUT₁

INPUT₂   27

MASS CODING PROCESS

17

COMPUTER, DIGITAL OR
ANALOG PROCESS

OUTPUT₂

MASS CODED SETS OF PERIPHERAL
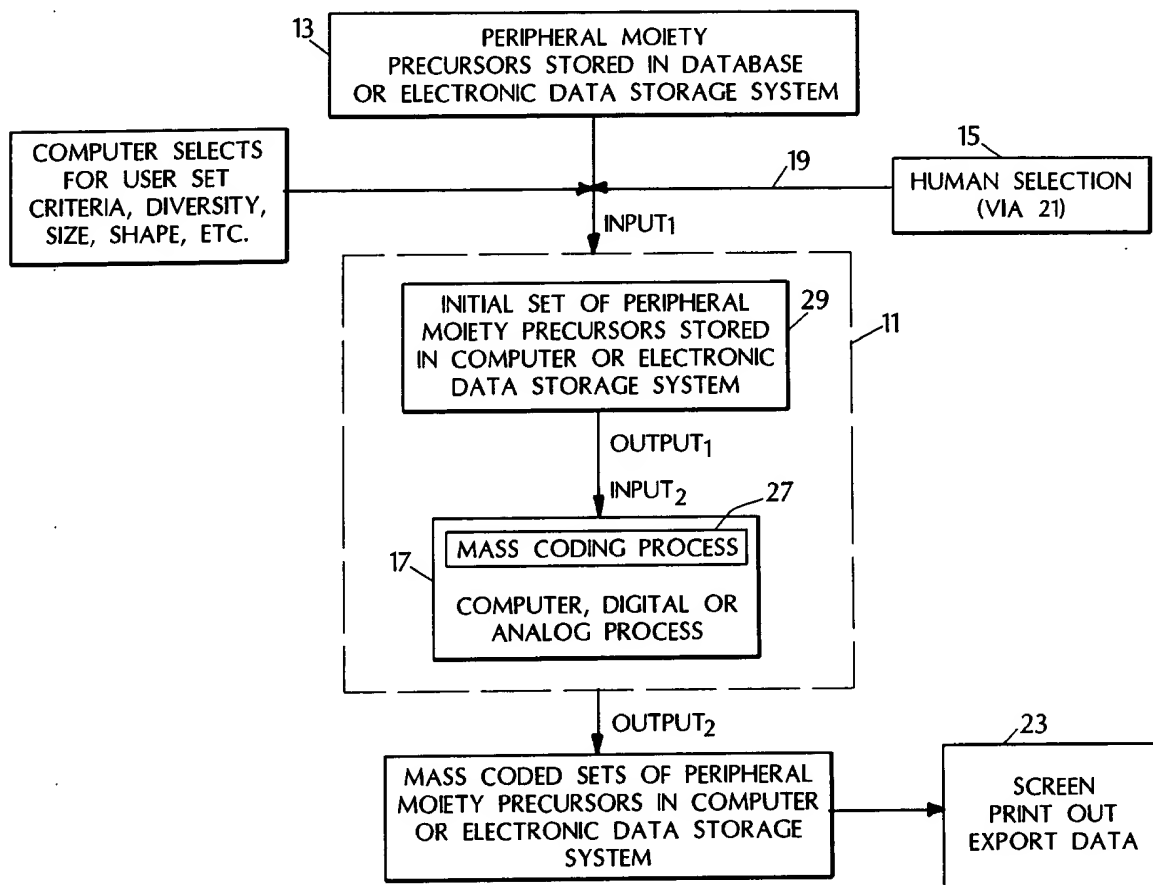MOIETY PRECURSORS IN COMPUTER
OR ELECTRONIC DATA STORAGE
SYSTEM

23
SCREEN
PRINT OUT
EXPORT DATA

SYSTEM FLOW FOR
MASS CODING PROCESS

FIG. 3